Roadmap
for
Process Equipment
Materials Technology

October 2003

Preface

Today's globally competitive marketplace presents enormous challenges to the chemical industry and the basic industries that rely on chemical processes, such as wood pulping, petroleum refining, and pharmaceuticals. Chemical industries must compete in terms of economics and product performance, while balancing the cost of environmental stewardship and social equity. The consumption and cost of resources, from labor to energy to raw materials, plays a key role in maintaining this balance.

Even in today's high technology world, heavy manufacturing equipment crafted from steel, refractories, concrete and other engineered materials forms the core of these vital industries. How well these materials of construction perform, and subsequently the reliability of the equipment, can make the difference between turning out a competitive product and losing market share. Materials of construction play a critical role in operational and workplace safety, and are a key factor in environmental compliance (containment of process fluids).

Today's materials of construction have evolved dramatically since the industrial age, in response to industry's changing demands for materials. Changes in the way products are manufactured, the type of raw materials used, and environmental concerns create needs for new and better materials. While today's materials are better than ever, they are still challenged by environmental degradation (e.g., corrosion), limited or uncertain performance in severe conditions, and a limited lifetime of usefulness. Our less than complete knowledge of the fundamental science of materials degradation, and inadequate technology for monitoring and predicting material performance are also limiting factors.

The end result is a tremendous cost burden to industry for maintenance and operation of vital processing equipment. For example, the total direct cost of materials corrosion to production and manufacturing industries is nearly $18 billion annually; the total national cost in all sectors of the economy is over $275 billion [*Corrosion Costs and Preventive Strategies in the United States*, NACE International, 2003]. Costs are incurred due to disruption in supply of product, lower product yields, loss of reliability, lost capital, and resource costs related to corrosion management.

This *Technology Roadmap* addresses the ever-changing material needs of the chemical and allied process industries, and the energy, economic and environmental burdens associated with corrosion and other materials performance and lifetime issues. While technology exists to reduce or mitigate corrosion, considering the current cost burden to industry, there is substantial opportunity for improvement. Research and development is needed to create new solutions and materials that will reduce equipment failures, lengthen the time between equipment shutdowns, lengthen operating life, and subsequently reduce the use of energy and other raw materials. This *Technology Roadmap* outlines the most critical of these R&D needs, and how they can impact the challenges facing today's materials of construction.

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Executive Summary

In 1998 the Materials Technology Institute, Inc. (MTI) published the *Technology Roadmap for Materials of Construction, Operation and Maintenance in the Chemical Process Industry* to address some of the technology needs called out in *Technology Vision 2020: The U.S. Chemical Industry*. This document identified materials technology as a key area impacting the future economic performance and growth of the chemical process industries. In November 2002, MTI and the U.S. Department of Energy supported a workshop to update the original technology roadmap and respond to emerging trends and technical needs. The results of that workshop are reflected in this *MTI Roadmap for Process Equipment Materials Technology.*

Table ES-1 Performance Targets for Materials of Construction for 2020

- Reduce overall life-cycle costs of process equipment and infrastructure by 30%
- Reduce energy consumption by 30%
- Increase productivity of assets by reducing downtime by 25%
- Capture existing knowledge and effectively train a future workforce
- Protect the environment by
  - Containing processes and preventing unacceptable leakage and emissions
  - Recycling 95% of metallic materials of construction at the end of their useful life
  - Striving to select materials that ultimately reduce environmental impacts from processing operations
- Provide a safe operating environment through zero on-the-job

Performance Targets

Performance targets defined in the first *Roadmap* were updated and expanded to more clearly represent the goals for today's chemical and allied process industries (see Table ES-1). These reflect the continuing need to reduce costs, improve productivity, optimize resources, protect the environment, and ensure safe operating conditions. Capturing the knowledge embedded in today's materials science community and ensuring the availability of a future skilled workforce is an underlying and important goal.

Priority Research Needs

New priority research needs were identified based on today's changing industry and predicted future material needs. A number of key priority research topics emerged (see Table ES-2). These critical research areas focus primarily on improving the knowledge available to material engineers and scientists, enabling improved predictive capabilities for design and for condition assessment, and developing new materials that will meet the dynamic process challenges of the future.

Table ES-2 Selected Priority R&D Topics			
Knowledge Management *(collection, assessment, organization, delivery and use of materials information)*	**Prediction of Materials Degradation** *(how quickly and severely a material is degrading)*	**Condition Assessment and the Effects of Design, Fabrication & Maintenance on Asset Integrity** *(optimized equipment integrity)*	**New Materials for Challenging Process Conditions** *(materials for new processes, e.g., smaller-footprint plants, alternative/ heavier feedstocks, new media)*
Smart systems (materials database, conversational query capability, integration of Masters knowledge)

New/improved materials models (Entirely new data and models; thermophysical, thermodynamic, thermochemical, thermomechanical, kinetic, corrosion, wear and stress; | **Data and model development** (collection and integration of materials environment/ performance data – see Grand Challenge)

Standard polymer formulations (identifying best standard polymer formulations for polymer degradation data in specified environments) | **Automated fitting and joining of materials** (techniques for metals and non-metals, custom fabrication, automated welding)

Basic materials interactions in the physical environment (models for optimizing composition of corrosion-resistant metals and non-metals, models for materials degradation, combined data | **Accelerated testing of materials** (detect and measure extrapolatable data in the lab, easily achieved lab test conditions)

Materials sustaining protective layers at high temperatures (corrosion resistance in range 350-750°C)

Smart materials (materials with detectable property changes, self-healing or protecting) |

stand alone and integrated models)		for metal corrosion and non-metal degradation)	**Corrosion protection for carbon steel** (cladding and surface treatments)

Grand Challenges

Many of the priority R&D topics identified cut across several technical areas, and to effectively address these needs a set of "grand challenges" were developed. These grand challenges are large, integrated, multi-partner, multi-disciplinary R&D activities that incorporate more than one R&D element but strive to achieve a single broad goal. Through these grand challenges valuable partnerships can be established that leverage public and private sector resources and serve to accelerate high-value research that could not otherwise be accomplished by a single firm. Table ES-3 outlines the key focus areas for the grand challenges.

<div align="center">Table ES-3 Grand Challenges</div>

Delivery of Materials Engineering Information	Modeling and Prediction of Materials Performance	Condition Assessment
Centralized information system with comprehensive, standardized, refereed data and tools, linked to and compatible with external tools and models. Incorporates a search engine and provides advice for materials selection and data mining.	Capability to predict the corrosion behavior of all materials (metals, polymers, reinforced composites, filled polymers, ceramics) over time, including chemistry, effects of composition, and degradation mechanisms.	Non-invasive, remote, real-time and on-line inspection methods for equipment conditions or to measure equipment integrity. Methods should allow remote understanding of physical/ mechanical condition, use see-through vessel and pipe imaging, and have the ability to flag damaging process conditions.
Key R&D Elements • International literature surveys • Data collection/collation • System structure development – software, hardware, system schematic • Data links with different disciplines • Definition of customer needs • Guidelines/rules for acceptable data • Platforms for data integration	**Key R&D Elements** • Fundamental chemistry and thermodynamic models • Models for corrosion resistance of alloys • Fundamental understanding of corrosion, stress cracking, coking • Non-destructive evaluation methods • Fast, high precision measurement of property changes in non-metals • Measurement/prediction of defect propagation • Fitness for service evaluation tools	**Key R&D Elements** • Cost-effective technologies for on-line, non-intrusive, non-destructive evaluation of materials (see-through assessments, modification of existing full-vessel imaging, evaluation of wall loss, cracking, materials property degradation for primary pressure vessels) • On-line sensors for detection of high temperature metal loss
Benefits LOW ———————————— HIGH Energy ▮▮▮▮ Environment ▮▮▮▮▮▮▮ Yield ▮▮▮▮▮▮ Safety and Reliability ▮▮▮▮▮	**Benefits** LOW ———————————— HIGH Energy (mid-high) ▮▮▮▮▮▮ Environment ▮▮▮▮▮▮▮ Yield ▮▮▮▮▮▮▮ Safety, Competitiveness, Flexibility, Reliability ▮▮▮▮▮▮▮	**Benefits** LOW ———————————— HIGH Energy ▮▮▮▮▮▮ Environment ▮▮▮▮▮▮▮▮ Yield ▮▮▮▮ Safety and Reliability ▮▮▮▮▮▮▮

The Path Forward

MTI intends to use this roadmap to develop project proposals during the years 2003-2006. It is also hoped that the priority needs identified in this roadmap will provide guidance for public and private decision-makers in supporting these and parallel research efforts in materials science and engineering. Through research in priority areas, progress can be made toward the goals that have been defined for this technology roadmap, and which are critical to the future

competitiveness of the chemical and allied process industries. Multi-faceted research partnerships that include industry, government, national laboratories and universities will be key to accelerating R&D and leveraging limited resources for high risk materials research that yields significant benefits to both industry and their respective nations.

1 Overview

Background

In 1996, the chemical industry prepared a vision of how it would meet its competitive challenges over the next two decades. *Technology Vision 2020: The U.S. Chemical Industry* described the current state of the industry, a vision for the future, and the technical advances that would be needed to make this vision a reality. Materials technology was identified in *Vision 2020* as a key area that will help determine the future economic performance and growth of the chemical process industries. Materials of construction comprise the physical infrastructure within the chemical and allied process industries. Materials are critical to industry competitiveness, and also contribute to the economic viability of many other industries that rely on chemical products.

In 1998, the Materials Technology Institute of the Chemical Process Industries, Inc. (MTI) collaborated with the U.S. Department of Energy (DOE) to develop a technology roadmap that would address the materials technology solutions called for in *Vision 2020*. This effort resulted in the publication of the *Technology Roadmap for Materials of Construction, Operation and Maintenance in the Chemical Process Industry*. After the publication of the Roadmap, MTI developed more than 20 ideas for projects to address defined needs and prioritized them. Subsequent funding of the five highest priority projects delivered practical, useful information to MTI and chemical process companies worldwide.

Technology needs and the challenges facing the chemical process industries are dynamic. For example, growing interest in biological processes, nanotechnologies, and hydrogen fuels are creating new technology opportunities along with new demands for materials of construction. In November 2002, MTI and DOE supported another workshop to update the original technology roadmap and respond to emerging trends and technical needs. The results of the workshop are reflected in this updated *2003 MTI Technology Roadmap for Process Equipment Materials Technology*.

Trends Impacting Materials of Construction

Energy
Over the next decade, the fuel choices available to chemical manufacturers will be changing. Energy sources such as biofuels, hydrogen and modular power (small, mobile onsite power units) will be increasingly available. Volatility in energy prices and availability will drive users towards energy conservation and increasing use of byproduct and waste heat sources.

Environment
Tighter environmental regulation of air emissions (combustion and fugitive) and hazardous effluents will continue to influence material choices. There are increasing trends toward sustainability in manufacturing and the generation of fewer carbon emissions, and the impacts of policies in these areas will be felt in materials selection and design of equipment. Material choices will increasingly reflect sustainability and capability for recycling. While recycling of nickel-based materials and stainless steel is widely done today, many opportunities are not taken advantage of due to technical or other limitations.

New Materials

Many new materials are on the horizon and may find application as materials of construction. This includes the use of ceramic materials in polymers, compound materials, and coatings. Nanotechnology and other technological advances may lead to entirely new concepts in materials technology. The emergence of "smart" materials (self-repairing) could have significant impacts on materials of construction and equipment maintenance.

Information Technology

The enormous resources of the Internet, increasing computing and simulation capabilities, and the growing availability of data will influence both materials design and selection. The growing need for information on a round-the-clock basis in real-time will change how data is collected, stored and shared. Newly available data may need to be validated to establish its usefulness.

Workforce

Changing materials requirements will increasingly require multidisciplinary expertise beyond traditional materials science and engineering. However, while demand is increasing, the workforce and leadership knowledgeable in materials science is shrinking. Knowledge resides with "Masters", and fewer scientists and engineers with an interest in materials are entering the workforce. Slowing the development of the next generation of knowledge will ultimately impact the ability to design, select and evaluate materials effectively.

Global Economics

The globalization of the chemical and allied process industries has already impacted materials design, selection and manufacture. Manufacturing operations are moving overseas and material fabricators are globally dispersed. International competition is also driving a lower cost structure in industrialized countries.

Process Conditions

Materials of construction play a key role in manufacturing companies' drive to increase operational reliability at low cost. More severe operating conditions (higher temperatures, pressures, increased throughput) and the emergence of new processes (supercritical fluids, plasmas, nanoprocesses, bioprocesses) will require new materials and equipment designs.

Overall Performance Targets

The updated performance targets for materials of construction are shown in Figure 1-1. These goals build on and redefine those developed in the 1998 *Technology Roadmap*.

Figure 1-1 Performance Targets for Materials of Construction for 2020

Reduce life-cycle costs of process equipment and infrastructure by 30%

Reduce energy consumption by 30%

Increase productivity of assets by reducing downtime by 25%

Capture existing knowledge and effectively train a future workforce

Develop capacity to respond to new challenges

Protect the environment by
- Containing processes, preventing unacceptable leakage and emissions
- Recycling 95% of metallic materials of construction at the end of their useful life
- Striving to select materials with decreased environmental impacts

Provide a safe operating environment through zero on-the-job injuries and a secure plant

2 Knowledge Management

Definitions for Knowledge Management

KM needs – continuous improvement that identifies emerging or critical technical programs/support systems to enhance individual and network capability.

Moogle – google-type Internet search engine for materials data and information.

Smart System – capability that enables non-specialists to excavate levels of knowledge developed by practical subject matter experts using frequently answered question sets and similar logic that enhances information gleaned from data alone.

Data – qualitative, quantitative, and semi-quantitative information that an end-user draws on to make judgments, and which must be properly filtered to be of practical value.

Organized knowledge – Data, models, Moogle, smart systems turned to technical or business advantage

Action – end product of knowledge: decisions that influence the selection of technical options or the conduct of business.

Knowledge management (KM) involves the gathering, assessment, organization, delivery and use of materials-related information. The knowledge management process can be defined in terms of three interacting groups: leaders ("technical masters" with knowledge), feeders (providing data and other input), and needers (end-users).

Broad issues surrounding knowledge management include the effective development and application of KM; acquiring tacit and explicit knowledge; developing the information and knowledge required; making information accessible and easily extractable; managing the content; and integrating knowledge into decision-making.

Performance Targets

Table 2-1 Knowledge Management Performance Targets
- Reduce time to access/search information
- Increase availability and exchange of information/knowledge
- Improve the quality of information/KM
- Optimize decision making
- Reduce the cost of obtaining data

Performance targets for knowledge management are shown in Table 2-1. These reflect the current deficiencies in KM systems and especially the need to improve not just the quality of data but the accessibility and utility of information.

Technical Challenges

The top technical challenges for knowledge management are shown in Table 2-2. These are the critical limitations that must be addressed by R&D to enable the development of more useful and complete knowledge management systems.

Table 2-2 Technical Challenges for Knowledge Management

Table 2-2 Technical Challenges for Knowledge Management
Data/Information Quality
Continued use of obsolete, proprietary, non-reviewed (peer), or partial data
Language/Terminology Problems
Language and cultural diversity, globally and locally (i.e., different classes, generations, or functional groups may interpret data differently)
Knowledge Infrastructures
• Knowledge of technical masters leaving the industry is not being captured • Need to create and utilize multidisciplinary networks of people/facilities • Variance in company needs and industry needs
IT and Software Issues
• Changes in IT and software • Need to design, build, and maintain high quality software tools
Relevancy and Value of Data Information
• Uncertainty about the validity, sensitivity and accuracy of data
Transfer and Exchange of Information
• Understanding how knowledge sharing networks are conceived and maintained

Priority Research Needs for Knowledge Management

The priority research needs for knowledge management are shown in Table 2-3. The highest priority is the development of smart systems that link data and experience to create an expert system of knowledge. This is a mid-long term activity that could take from 3-10 years to accomplish. In the near term, high priorities include optimizing the use of intranet and Internet search engines, developing guidelines for acceptable data, and identifying existing databases that contain accurate and reputable information. Details on the highest priority research areas are provided on the following pages. The connections between R&D and supporting activities are shown in Figure 2-1 (page 5).

Some of the research needs shown here have been incorporated into a larger, integrated "grand challenge" for delivery of materials engineering information. The details of this grand challenge are outlined in Chapter 6.

Table 2-3 Priority R&D Needs Identified for Knowledge Management						
Top priority R&D = ✪; Priority R&D = —						
	Smart Networks and Systems	**On-line Search Tools**	**Sharing Information**	**Define User Needs**	**Data Quality**	**Modeling and Software**
Near Term (0-3 Years)	• Develop a system whereby complex information can be "layered" to expose deeper and deeper levels of tacit knowledge ✪ • Conduct behavioral research to optimize effectiveness of networks ✪ • Find/develop software to support networks —	• Moogle! - "Google" of materials engine information ✪ • Identify/list "good" databases, searchable databases (stamp of approval) ✪	• Develop new approaches to sharing information during the introduction of a new chemical process ✪	• Survey "needers" to learn 80% of their daily information requirements ✪	• Develop a list of rules/ guidelines for acceptable data ✪	• Develop readily available non-proprietary case studies demonstrating the use of software tools —

		Table 2-3 Priority R&D Needs Identified for Knowledge Management				
		Top priority R&D = ✪; Priority R&D = —				
	Smart Networks and Systems	On-line Search Tools	Sharing Information	Define User Needs	Data Quality	Modeling and Software
Mid Term (3- 10 Years)	• Develop smart system that links data to "master" experience to create knowledge ✪ — multidisciplinary pool — develop heuristic database — improve decision making • Implement system where complex information can be "layered" to expose deeper levels of tacit knowledge ✪					• Develop smart and flexible software database that would also allow masters to document their knowledge —
Long Term (> 10 years)						• Develop new/improved materials models that use new knowledge — — use models to define new data needs

			NETWORKS Development of optimum networks of end-users

"MOOGLE" Google-type Internet search engine for materials data and information	SMART SYSTEMS System that links data with "Masters" experience to provide knowledge and insight	PROBLEM SOLVING Shared approaches to overcoming specific-materials- related challenges	KM NEEDS Understanding and characterization of user KM needs

MODELS Development of new and improved knowledge- based materials simulation tools	DATA Guidelines, process and rules for approved/verified data	ACTION Feedback to all of the above

ORGANIZED KNOWLEDGE
Materials selection, reliability
improvement, best practices,
condition assessment, and
distribution of knowledge

Applying knowledge to solve problems

**Figure 2-1 Linkages for R&D and Other Activities
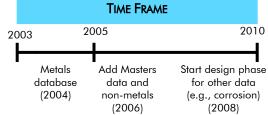in Knowledge Management**

PRIORITY RESEARCH AREA

Smart System

Key Technical Elements
- Material database (e.g., metals, non-metals, all relation properties)
- Capability for conversational style of questions and answers
- Methodology for integrating Masters knowledge

RISK

LOW   HIGH

Technical Risk

Difficult to extract tacit knowledge from Masters and integrate with database

Commercial Risk

Requires no interruption in production

BENEFITS

LOW   HIGH

Energy

Environment

Yield

Higher Quality Solutions

TIME FRAME

2003   2005   2010

Metals database (2004)

Add Masters data and non-metals (2006)

Start design phase for other data (e.g., corrosion) (2008)

Ongoing maintenance and data expansion

Research Pathway

Research is needed to develop a smart system that mimics how a Master combines data and experience to provide materials-related answers. The system should rely on a multidisciplinary pool of expertise and data, include a heuristic database, and improve decision-making. The proposed effort will start with a metals database and progress to the addition of Masters knowledge and non-metals within 2-3 years. Industry and national labs will provide data, Masters, rules/guidelines, and certification. Universities will participate by developing approaches and methodologies. There is a role for Government funding for non-

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PRIORITY RESEARCH AREA

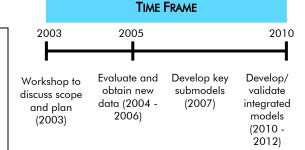### New/Improved Materials Models

Key Technical Elements
- Thermophysical, thermodynamic, thermochemical, thermomechanical, kinetic, corrosion, wear and stress
- Stand-alone and integrated models
- Evaluation of current data
- Development/validation of entirely

RISK

LOW   HIGH

Technical Risk

High for integrated models, medium for individual models

Commercial Risk

Driven by industry desire to buy/use tools with greater accuracy and speed

BENEFITS

LOW   HIGH

Energy

Environmental

Yield

Safety, Life Cycle Costs

TIME FRAME

2003   2005   2010

Workshop to discuss scope and plan (2003)

Evaluate and obtain new data (2004 - 2006)

Develop key submodels (2007)

Develop/ validate integrated models (2010 - 2012)

Research Pathway

Research is needed to develop new integrated models to solve technical problems. New sets of data will be needed to support these models. Validation of new data sets and accompanying models will be critical to this effort. Data and model validation are envisioned as a collaborative activity involving equipment suppliers, the chemical industry, national laboratories and universities. Model development would be conducted at national laboratories and universities. R&D could be cost-shared among suppliers, industry and government.

3 Prediction of Materials Degradation

Background

Prediction of materials degradation is critical to optimizing maintenance schedules, reducing downtime, and mitigating the risk of equipment failure. By predicting how quickly and how severely a material is degrading, plant engineers can determine when to inspect, replace or how to maintain equipment within a reasonable safety margin.   A key component is the development of better methods for predicting corrosion performance, which can be accomplished by exploring technologies and opportunity areas that may be able to reduce cost and failure risk.

Performance Targets

Performance targets for prediction of materials degradation are shown in Table 3-1. Achieving these targets will substantially improve the ability of plant engineers to predict how materials behave and degrade over time, and will move the industry toward real-time monitoring of equipment conditions. The end result will be lower costs for maintenance and equipment repair, better equipment design capability, reduced risk of catastrophic failure, and fewer disruptions in production.

Table 3-1 Performance Targets for Prediction of Materials Degradation

- Predict the performance of any metal alloy in any environment (using software calculations or logic method)
- Predict the performance of non-metals in a short time period (hours)
- Complete move from calendar-based inspection to risk (knowledge)-based inspection and from design code-based acceptance to rigorous fitness-for-service (e.g., FEA) methods
- Achieve ability to continuously monitor in-situ for degradation
- Compile and integrate user-friendly database for degradation of non-metals
- Ensure availability of dynamic materials (e.g., materials that get stronger under stress, materials that "heal" scratched surfaces, coatings that self-heal or emit a signal when breached)

Technical Challenges

The technical challenges to effective prediction of materials degradation are shown in Table 3-2. Computational capability, the lack of non-intrusive measurement technology, and incomplete or non-standard data are all significantly limiting factors in the development of better predictive tools.

Table 3-2 Technical Challenges for Prediction of Materials Degradation

Multidisciplinary Modeling

- Inadequate computational power (computational fluid dynamics, finite element analysis)
- Insufficient computation capability to connect process design software to thermodynamic calculation modeling/ kinetic software

Non-metals

- Polymers: must know part's composition to predict performance
- Industry does not use standard polymer formulations for testing and comparison of data
- Lack of technology to allow rapid evaluation of non-metallics' performance

Fundamental Knowledge

- Lack of cost-effective technologies and methods for on-line, non-intrusive evaluation of materials degradation in situ
- Inadequate dynamic risk management techniques

Data

- Lack of standard format for presenting data and methods
- Lack of data to predict alloy performance and/or degradation rate (e.g., lack of complete collection of thermodynamic and kinetic data for alloys and corrosives)

Priority Research Needs for Prediction of Materials Degradation

Priority research needs for prediction of materials degradation are illustrated in Table 3-3. The highest priority overall is the collection, collation, and integration of materials and environmental performance data to support future model development. This is a near-term, ongoing activity that will continue over the mid- to long-term as new materials are developed and put in use. Another near-term priority that is necessary to the data effort is the development of on-line sensors to detect high temperature metal loss and monitor fouling. Over the mid-term, a critical need is to expand the utility of alloy corrosion models to include additional elements such as localized corrosion. Validation is a key part of model development and model reliability.

Because of the importance of this topic, and the significant impact it can have on materials design and use, an integrated effort for prediction of materials degradation is outlined in Chapter 6 as a "grand challenge" (Modeling and Prediction of Materials Performance). This integrated effort combines much of the highest priority R&D identified here, as well as supporting research in fundamental materials science. A diagram of how the important R&D and other activities link together is shown in Figure 3-1 (page 9).

Identifying the best standard polymer formulations in specified environments is another high priority. Formulations would be classified as a function of hardness, minimum and maximum temperatures, and lifetime. Degradation data would be oriented for these standard formulations.

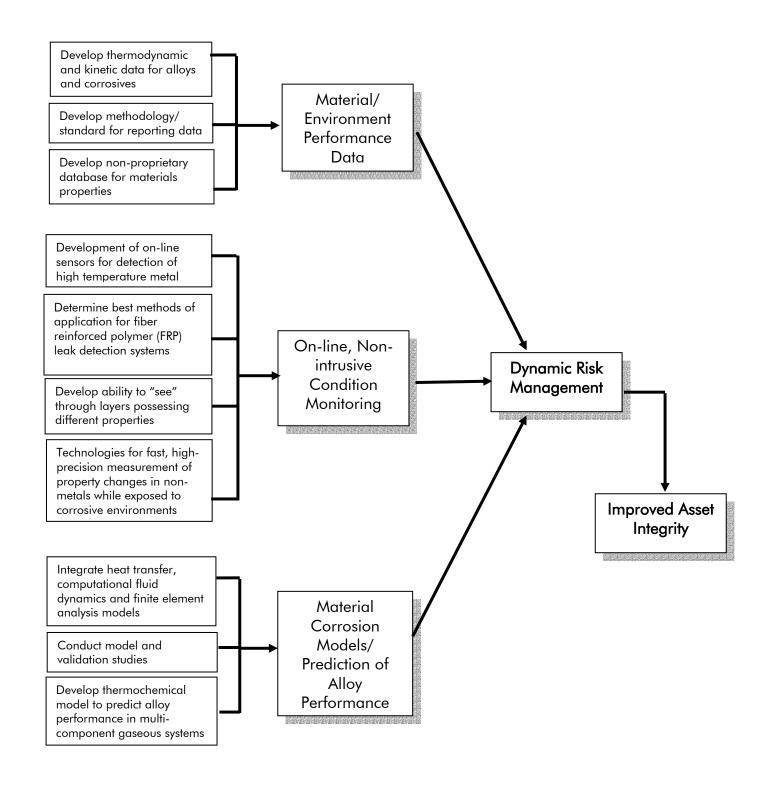| Table 3-3 Priority R&D Needs Identified for Prediction of Materials Degradation			
Top priority R&D = ✪; Priority R&D = —			
	Validation/ Implementation	Monitoring/Measurement Technologies	Data and Model Development
Near Term (0-3 Years)	• Develop improved dynamic risk management techniques — • Connect heat transfer CFD and FEA models — — aqueous — non-aqueous	• Develop on-line sensors for detection of high temperature metal loss due to fouling ✪ • Determine best methods of application for fiber-reinforced polymer (FRP) leak detection systems, including existing technologies — • Monitor for fouling	• Continue integration of materials/environment performance data collection/collation (ongoing activity) ✪ • Develop thermodynamic data for alloys and corrosives (validate in mid-term) —
Mid Term (3-10 Years)	• Develop approaches to determine long-term cost of ownership issues/evaluation ✪ • Identify "best" standard polymer formulation for each family ✪ • Fund demonstration projects that apply and illustrate improved materials and integrity management in process plants —	• Develop cost-effective technologies and methods for online, non-intrusive evaluations of materials ✪ • Develop technologies for fast, high-precision measurement of property changes in non-metals while exposed to corrosive environments — • Develop ability to "see" through layers possessing different properties —	• Expand range of utility of alloy corrosion models ✪ • Validate thermodynamic data for alloys and corrosives —

Figure 3-1   Linkages for R&D and Other Activities in
Prediction of Materials Degradation

4 Condition Assessment and the Effects of Design, Fabrication, and Maintenance Practices on Asset

Background

Design, fabrication and maintenance directly impact both the performance and integrity of equipment over its lifetime. The focus here is to explore condition assessment, design, and repair practices that will ensure optimum equipment integrity. This includes fabrication technology, inspection, repair technology and practices, and data that will influence codes and standards.

Performance Targets

Performance targets for condition assessment and the design, fabrication, inspection and maintenance of equipment are shown in Table 4-1. These goals illustrate the wide-reaching impact that improved design and fabrication processes can have on equipment integrity. Inspection of equipment condition is a key element. Non-intrusive, reliable inspection techniques will help to reduce unplanned outages and equipment shutdowns; these are often the root cause of emissions and materials degradation.

Table 4-1 Performance Targets for Condition Assessment and Design, Fabrication and Maintenance Practices

- Reduce manpower required for the design/build/fabrication process by 20% by 2020, without compromising quality
- Develop more analytical approaches (analysis-based codes) for design/build than those in current codes
- Increase fabrication productivity by 30% through more effective design/build/fabrication of equipment
- Optimize resources required for inspection
- Reduce downtime caused by unforeseen failures by 80%
- Reduce intrusive inspections by 60% or more
- Achieve timely training and education in materials design/build/inspection across industries,

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Technical Challenges

The technical challenges for condition assessment, design, fabrication and maintenance are shown in Table 4-2. Inadequate sensor technology and the lack of effective non-intrusive methods for assessing internal equipment conditions continue to limit the effectiveness of inspection processes.

Table 4-2 Technical Challenges for Condition Assessment and Design, Fabrication, and Maintenance Practices

Inspection Optimization
• In service sensors as well as non-intrusive sensors can miss conditions and give false calls
• Insufficient technology and methods to quantify internal equipment conditions without entering
Fundamental Understanding
• Lack of understanding of materials degradation
• Lack of access to materials data by plant designers
Training/Skilled Workforce
• Lack of time to transfer knowledge to new generation
• Lack of skilled workers, designers, fabricators

Priority Research Needs for Condition Assessment and Design, Fabrication and Maintenance Practices
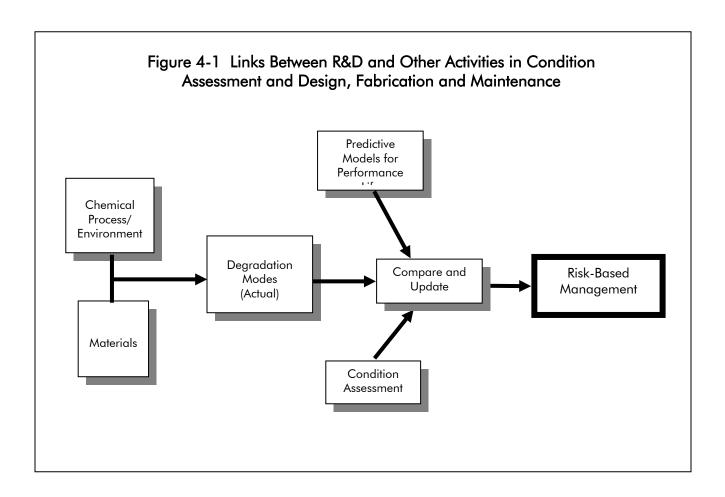
The priority research needs for condition assessment and design, fabrication and maintenance are shown in Table 4-3. In the area of inspection, the highest priorities are to develop non-destructive technology to monitor the internal condition of equipment. A comprehensive and multiple-partner effort in condition assessment was identified as a top priority, and is outlined as a Grand Challenge in Chapter 6.

In design and fabrication, new technologies such as automated joining as well as better design codes and guidelines are high priorities. A key challenge is to better understand basic materials degradation in the physical operating environment. Integrated R&D programs for both of these areas are described on the following pages. The links between R&D activities are illustrated in Figure 4-1.

Table 4-3 Priority Research Needs for Condition Assessment and Design, Fabrication and Maintenance Practices Top priority R&D = ✪; Priority R&D = —					
Time Frame	Degradation Modes	Education/ Training	Inspection Optimization	Design/Fabrication Materials and Methods	Information Management/ Dissemination
Near Term (0-3 years)		• Transfer common knowledge (fabrication, corrosion, etc.) at national level to avoid reinventing the wheel ✪	• Develop improved in-service corrosion sensors ✪ • Conduct large demonstration project to show effective inspection program and corrosion control ✪ — Comparing old/new methods in terms of cost, technology		

| | | | | Design/Fabrication | Information |
Time Frame	Degradation Modes	Education/ Training	Inspection Optimization	Materials and Methods	Management/ Dissemination

Table 4-3 Priority Research Needs for Condition Assessment and Design, Fabrication and Maintenance Practices
Top priority R&D = ✪; Priority R&D = —

Time Frame	Degradation Modes	Education/ Training	Inspection Optimization	Design/Fabrication Materials and Methods	Information Management/ Dissemination
Mid Term (3-10 years)	• Combine metal corrosion data with nonmetal materials degradation data for same conditions — • Integrate experimental process data with sensor data —	• Establish reliability Certification Program; training in remaining life assessment ✪	• Develop NDE technology that allows external assessment of internal corrosion conditions ✪ • Modify existing equipment for full-vessel imaging (now available for transport, now used for homeland security) ✪ • Develop new in-service corrosion sensors ✪ • Create multi-disciplinary National Center (led by university or national lab) for sensors ✪ • Obtain good performance data on existing and emerging NDE technologies —	• Develop automated welding processes for in and out of position welding (considering out of round objects) ✪ (Mid-Long Term) • Create analysis-based design codes (similar to European codes) ✪ • Establish guidelines for critical issues in fabrication and inspection quality —	• Create central database for existing equipment (failure histories, corrosion, effectiveness of inspections) ✪
Long Term (>10 years)			• Develop fundamental models for optimizing the composition and properties of corrosion-resistant materials (metals and nonmetals) for specific environments ✪		

Figure 4-1 Links Between R&D and Other Activities in Condition
Assessment and Design, Fabrication and Maintenance

Priority Research Areas
Condition Assessment and the Effects of Design,
Fabrication and Maintenance Practices on Asset

PRIORITY RESEARCH AREA

Automated Fitting and Joining of Materials

Key Technical Elements
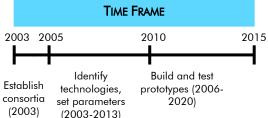- Techniques for all materials (metals and non-metals)
- Methods for custom fabrication
- Automated welding processes

RISK

LOW	HIGH

Technical Risk

Requires combination of adaptive control, welding, and robotics

Commercial Risk

Could be affected by low-wage foreign resources

BENEFITS

LOW	HIGH

Energy

Yield

Product Reliability

Research Pathway
Research is needed to develop new methods for automated fitting of and joining of materials. A key research component is automated welding processes for in and out of position welding. The proposed effort would start with establishing a cross-disciplinary consortia (welding, controls, alloys) with participants from industry, government, national labs, and universities. R&D steps include identification of key technologies, selection of materials to focus on, and prototype construction, design and testing. Commercialization of new technology could occur within 6-

TIME FRAME

2003 2005   2010   2015

Establish consortia (2003)

Identify technologies, set parameters (2003-2013)

Build and test prototypes (2006-2020)

PRIORITY RESEARCH AREA

Basic Materials Interactions in the Physical Environment

Key Technical Elements
- Fundamental models for optimizing composition of corrosion-resistant materials (metals and non-metals)
- Predictive models for materials degradation (e.g., by mode, important chemical processes, thermodynamics)
- Combined data for metal corrosion and non-metal degradation under same conditions

RISK

LOW	HIGH

Technical Risk

Limited understanding of corrosion, inability to solve some pitting problems

Commercial Risk

Improves material selection

BENEFITS

LOW	HIGH

Energy

Environmental

Yield

Safety, Reliability, Flexibility

Research Pathway
Research is needed to develop models to accurately simulate and predict corrosion and degradation modes in a variety of metals and non-metals, and under different process conditions. Near-term efforts will focus on identifying existing models and knowledge gaps. Focused R&D can then be conducted as a concerted effort between materials suppliers, universities and national labs.

TIME FRAME

2003 2005   2010   2015

Survey existing models, identify gaps, process (2003)

Conduct materials and laboratory research (2005 ➜)

5 New Materials for Challenging Process Conditions

Background

New materials are needed for chemical processing that can cost-effectively withstand challenging process environments. The focus is on both metals and non-metallic materials for new process challenges such as smaller-footprint plants, alternative (e.g., heavier) feedstocks, new reaction media (e.g., ionic liquids, supercritical fluids), biological processes in dilute media, more energy-efficient processes (higher/lower temperatures), and separations.

Performance Targets

Table 5-1 Performance Targets for New Materials
• Supply new materials that eliminate barriers to new chemical processes. This will be achieved through combinations of material properties such as strength, corrosion resistance, fabricability, wear resistance and permeation (of ceramics and plastics), and the time dependence of these characteristics. • Express materials performance in currencies understood by senior management. • Eliminate the failures that could have been prevented using existing knowledge and technology. • Develop methods to monitor continuously the rate of consumption of the remaining life of materials.

Performance targets for new materials are shown in Table 5-1. Achieving these goals will provide a new slate of more efficient materials of construction with improved properties and flexibility for many different applications. Development of new materials in combination with better understanding of materials life will enable equipment designers as well as end-users to make more informed, cost-effective and reliable decisions about materials selection and use.

Technical Challenges

The top technical challenges for new materials are shown in Table 5-2. Joining of new, advanced materials continues to be a significant challenge, along with ensuring that the joint exhibits properties similar to those of the parent materials. Developing new corrosion-resistant materials for high temperature processes is a key challenge that if overcome, could provide considerable energy and cost benefits.

Table 5-2 Technical Challenges for New Materials
New Materials Development
• Existing reinforcements for polymeric materials are limited to relatively low temperatures • New approach to wear resistance without sacrificing corrosion resistance
Testing of Materials
• Realistic test methods for materials selection
Joining and Fabrication of New Materials
• Joining of advanced materials (e.g., sealants, gaskets, welding) and ensuring joint has similar properties to bulk
Corrosion
• Resistance to water-side fouling and microbiological corrosion • Resistance to atmospheric corrosion and corrosion under insulation (without corrosion-resistant alloys)
Materials Utilization
• Ceramics are brittle and cannot be joined after casting
High Temperature Processes
• Corrosion-resistant materials for the temperature range 350-750°C needed to resist metal dusting and increase energy efficiency

Priority Research for New Materials

The priority research needs for new materials are shown in Table 5-3. A broad range of R&D will be needed to enable the development of new materials of construction, ranging from materials joining to better utilization and collection of materials design and performance data.   The highest priority topic areas include accelerated testing for all materials, manufacturing of materials with corrosion resistance in the high temperature range, corrosion protection methods for carbon steel, and development of smart materials. Details on these priority areas are provided on the following pages.

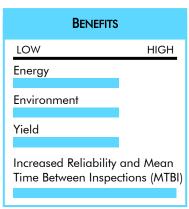| Table 5-3 Priority Research Needs for New Materials					
Top priority R&D = ✪; Priority R&D = —					
Time Frame	New Materials Development	Materials Processing, Joining and Surfacing	Fundamental Understanding	Testing	Data Mining/Modeling
Near Term (0-3 Years)		• Materials/surface treatment to avoid fouling without jeopardizing heat transfer)near-mid)— • Techniques for joining of alumina forming materials (near to mid) —	• Improved understanding of interactions of fouling and corrosion (near to mid) —	• Finite element modeling for polymer materials and verification by real life exposures in lab and field —	• Centralized database of materials properties on the Internet ✪
Mid Term (3-10 Years)	• Develop/demonstrate ceramic heat exchanger concepts ✪ • Apply existing knowledge (experimental design statistics) for efficient R&D — • Develop concrete with improved corrosion resistance (e.g., reinforcement, denser, coatings, etc.) — • New reinforcements/ fibers for polymeric composites — • Evaluate processes enabled by advanced materials (composites, intermetallics) —	• Explore economical corrosion protection methods for carbon steel (coatings, electrochemical) ✪ • Anti-coking and metal dusting-resistant coatings and alloys — • Inexpensive method for joining ODS (oxide dispersion strength) alloys — • Inexpensive method to clad corrosion-resistant metals on base metals — • Adhesives for corrosive environments —	• Manufacturing routes to materials that form protective layers in the temperature range 350-750°C versus high activities at high metal temperatures ✪	• Methodologies for accelerated corrosion testing (and integrate with modeling) including non-metallics — • Methodology of Arrhenius curves for accelerated testing for polymers — • Develop knowledge of creep of plastics over time in presence of chemicals	• Thorough literature search of existing knowledge – not just English; start with key topics, extend to many ✪ • State-of-the-art data compilations accessible via expert systems based on neural networks, available to designers —
Long Term (>10 Years)	• Develop smart materials that respond to changes in process conditions and develop self-protection — • Develop self-protection	• Weldable (joinable in field) ceramics ✪		• Lasers, microwaves and backscattering radiation as non-destructive, non-intrusive evaluation for polymers ✪	

PRIORITY RESEARCH AREA	RISK	BENEFITS

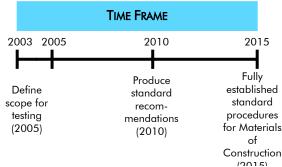### Accelerated Testing of Materials

Key Technical Elements
- Ability to detect and measure extrapolatable data in the lab in 24 hours to one week
- Test conditions that are easily achievable in the lab

RISK

LOW — HIGH

Technical Risk

Moderate

Commercial Risk

Easy to implement

BENEFITS

LOW — HIGH

Energy

Environment

Yield

Increased Reliability and Mean Time Between Inspections (MTBI)

Research Pathway

Research is needed to develop accelerated methods for testing of all materials of construction. The objective is reproducible measurements that can be accomplished as quickly as 24 hours in some cases. The proposed effort would begin with definition of scope – materials and formulations, chemicals, temperatures, and potential testing facilities. The goal is to have standard testing procedures defined within the next 7 years, and fully implemented in about 12 years.
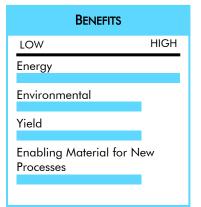
TIME FRAME

2003 2005 2010 2015

Define scope for testing (2005)

Produce standard recommendations (2010)

Fully established standard procedures for Materials of Construction (2015)

PRIORITY RESEARCH AREA	RISK	BENEFITS

Materials That Sustain Protective Layers at High Temperatures
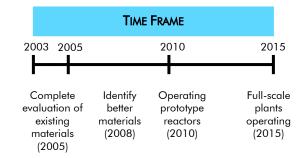
Key Technical Elements
- Corrosion resistance in the range of 350-750°C
- Applicability to steam reforming process
- Potential impacts on materials needs at the extremes – high and low temperatures
- Enabling critical processes (waste disposal, electricity generation)

RISK

LOW — HIGH

Technical Risk

Entirely new concepts are needed

Commercial Risk

Unproven technology

BENEFITS

LOW — HIGH

Energy

Environmental

Yield

Enabling Material for New Processes

Research Pathway

Research is needed to develop manufacturing routes to materials that effectively form protective layers in the temperature range of 350-750°C. Near-term efforts will focus on evaluating existing materials in-service, and then move on to developing and evaluating new materials. Within 10 years the objective is to design and develop prototype reactors with new materials that can be put into operation. Industry will evaluate existing materials, identify problems, set goals/targets, guide the project and build prototypes. National labs and universities will conduct fundamental work and devise innovative development approaches.
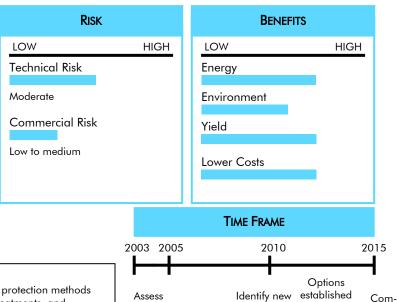
TIME FRAME

2003 2005 2010 2015

Complete evaluation of existing materials (2005)

Identify better materials (2008)

Operating prototype reactors (2010)

Full-scale plants operating (2015)

PRIORITY RESEARCH AREA	RISK	BENEFITS

Corrosion Protection for Carbon Steel, Cladding and Surface Treatments

Key Technical Elements
- Carbon steel that doesn't corrode or foul in low to medium corrosive environments
- Long lasting, cost-effective surfaces
- Draws on developments in nanotechnology and nanoprocessing

RISK

LOW — HIGH

Technical Risk

Moderate

Commercial Risk

Low to medium

BENEFITS

LOW — HIGH

Energy

Environment

Yield

Lower Costs

Research Pathway

Research is needed to develop new corrosion protection methods for carbon steel, corrosion-resistant surface treatments, and inexpensive methods to clad corrosion-resistant metal onto base metal. The proposed effort would begin by evaluating the current state-of-the-art, then move forward to identifying new options with commercial potential.

TIME FRAME

2003 2005   2010   2015

Assess state-of-the-art (2004)

Identify new potential options (2010)

Options established for commercial materials (2012)

Commercial Use (2017)

PRIORITY RESEARCH AREA	RISK	BENEFITS

Smart Materials

Key Technical Elements
- Identify means of signaling a change in material properties
- Identify sensing and signaling methods associated with property changes: Identify routes for material self-modification

RISK

LOW — HIGH

Technical Risk

Entirely new concepts to be developed

Commercial Risk

Medium to high

BENEFITS

LOW — HIGH

Energy

Environmental
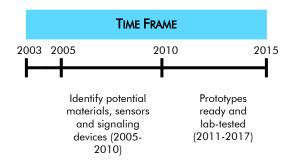
Yield

Research Pathway

Research is needed to develop "smart" materials that respond to changes in process conditions (e.g., self-healing and protecting). The two phases of R&D include development of sensing and signaling ability in materials, and incorporating the ability to self-correct and maintain the process. The early stages of research will involve identifying materials with detectable property changes, and parallel efforts to identify possible sensors and signaling devices. Prototypes could be available by 2011. National labs and universities will lead research; suppliers will provide samples for evaluation. Industry could commercialize technology by 2020.

TIME FRAME

2003 2005   2010   2015

Identify potential materials, sensors and signaling devices (2005-2010)

Prototypes ready and lab-tested (2011-2017)

6 Cross-Cutting Themes and Grand Challenges

Crosscutting Themes

A number of priority activities were identified that could impact many of the technical areas in materials engineering. These cross-cutting activities include research and development as well as financial tools, education and training.

Sensors
As shown in Table 6-1, sensors represent a key cross-cutting area for R&D.   New sensors will be critical for condition assessment as well as design of new materials, and could provide some of the data needed to support new modeling and predictive capabilities.   Priority activities are outlined for development of new sensors and modification of existing technology, including sensors currently used outside the chemical process industries. Entirely new concepts in sensing technology will be needed to make breakthroughs in inspection, monitoring, new materials design, and optimum operation and maintenance of equipment.

Table 6-1 Cross-cutting Themes		
Theme	Description	Proposed Priority Activities
Sensors	Sensors are needed for: • Corrosion • Chemical species • Self-diagnosis • Non-intrusive Inspection - detection of cracking inside pipes and vessels • Identifying where corrosion is occurring	• Define sensing requirements • Evaluate technology that is currently available and determine what can be adapted • Examine industries outside CPI to identify and adapt/modify sensing technology (e.g., medical, pharmaceutical, aerospace, nanotechnology, etc.) • Develop smart materials (embedded sensors) • Identify entirely new ways to sense (e.g., replace ultrasonics with a new method) • Develop technology for fast, high precision measurement of property changes • Conduct a demonstration project for new sensing technology • Utilize national labs/Lab Coordinating Council to accelerate R&D.
Information Delivery	See Grand Challenges	
Modeling	See Grand Challenges	
ND Methods	See Grand Challenges	
Cost of Ownership	Convince management of value of materials engineering by providing simple information on: • Life cycle costs • Capital costs • ROI, NPV, cash flow	• Provide tool for non-specialists to evaluate life cycle costs, energy costs, net present value, inspection costs (includes lifetime, specific materials). Must translate into financial language. Tool must have recognized "stamp of approval" • Tap the 3E+ program for insulation • Include ROR, ROI, NPV, cash flow analysis for short-term outlook • Ensure output is understandable by management
Education and Training	Fill the skilled work force gap, and capture the materials knowledge that is leaving the industry.	• Capture knowledge from Masters (materials selection advisors, "war stories") • Give MTI Fellows access to Forum discussions • Establish design guidelines and educational tools for working with new materials (design, joining and fabrication) • Offer scholarships for corrosion engineering and relevant fields

Education and Training

Education and training of the workforce and a loss of materials knowledge have been cited as key limiting factors in the future design, development and use of new materials of construction. There is a tremendous need to capture existing knowledge before it "retires" with the last generation workforce, and to expand the training of a new generation of materials scientists and engineers.

Cost of Ownership of Materials Engineering

Convincing upper management and R&D decision-makers of the potential cost benefits of materials engineering and using new materials is often difficult because the up-front investments are high and the returns are not easily understood. New tools are needed to enable management to evaluate the true costs and benefits accruing from an investment in new materials. These tools must incorporate life-cycle costs from cradle to grave, and translate the results into financial language that can be understood by senior managers as well as stockholders and investors.

Grand Challenges

A "grand challenge" can be described as a larger, high-value, high-risk multiple-partner and multi-disciplinary activity that incorporates more than one R&D element but strives to achieve a single broad goal. Valuable partnerships can be established through these grand challenges, and might include some combination of companies, trade groups, national laboratories, universities, government and private research institutes.

Three grand challenges have been identified which are of critical importance to materials of construction for the chemical and allied process industries. These essential research programs could have tremendous significance in terms of avoided energy costs, improved environmental performance, enhanced equipment reliability and performance, increased yield and productivity, and plant safety. The following pages describe the components of the three grand challenges, recommended partnerships, timeline for research, and the potential risks and benefits of each.

Grand Challenges
Condition Assessment
Modeling and Prediction of Materials Performance
Delivery of Materials Engineering Information

Some elements of the grand challenges may be found in other technical areas of this roadmap. However, the grand challenges outline a more concerted effort that brings together many essential R&D components under one umbrella. This integration provides the most opportunity to leverage limited funds as well as technical resources and maximizes the potential to accelerate critical research in materials science and engineering.

Condition Assessment

Inspection methods for evaluating the condition of process equipment are critical to efficient and safe plant operations, particularly as existing equipment ages. Conventional testing and inspection methods are frequently invasive and require a shutdown of the process. There is a tremendous need to move inspection processes away from "shut-down" mode and make them non-intrusive, real-time, remote, and on-line. Optimal inspection methods would allow non-intrusive understanding of mechanical and physical/chemical conditions of equipment, including see-through vessel and pipe imaging, and have the ability to flag potentially damaging process conditions. Ideally, an inspection system would not only flag potentially damaging conditions, but would provide an assessment of the

Technical Challenges

- Lack of reliable, cost-effective, on-line, self-sensing methods for corrosive conditions
- Limited effective non-destructive evaluation (NDE) technology
- Inability to non-intrusively inspect the interior of operating equipment, piping and associated

Key R&D Elements

- Cost-effective technologies for on-line, non-intrusive, non-destructive evaluation of materials
  - "See-through" external assessment of internal corrosion and equipment condition
  - Modification of existing technology for full-vessel imaging
  - Evaluation of wall loss, cracking, material degradation for primary pressure vessels (metal and non-metal), linings, coating and cladding
- On-line sensors for detection of high temperature metal loss
- Sensors for corrosion under insulation (CUI)

Partnership Roles and Responsibilities

Industry – Defines the problem, provides in-kind cost sharing

Government - Funds pre-competitive R&D (e.g., DOE, DoD)

National Labs - State-of-the-art resources accelerate R&D
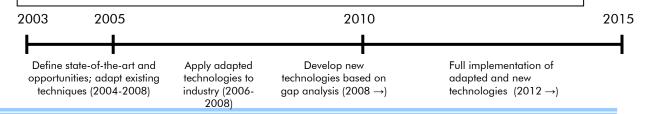
Universities - Conduct R&D, provide resources

RISK

LOW   HIGH

Technical Risk

Entirely new technology will be required.

Commercial Risk

Technology is easily retrofitted, with ample commercial markets.

BENEFITS

LOW   HIGH

Energy

Environment

Yield

Safety and Reliability

Research Pathway

In the near-term, research should be focused on evaluating and adapting existing techniques to the assessment of equipment conditions. In the mid-term, new techniques can be developed to address the remaining gaps in measurement technology. The goal is to have a suite of useful assessment technology that is commercially available within ten years. National labs and universities will have a key role in technology adaptation and development.

2003	2005	2010	2015

Define state-of-the-art and opportunities; adapt existing techniques (2004-2008)

Apply adapted technologies to industry (2006-2008)

Develop new technologies based on gap analysis (2008 →)

Full implementation of adapted and new technologies (2012 →)

Modeling and Prediction of Materials Performance

There is a critical need to develop the ability to predict the corrosion behavior of materials over time, including chemistry, effects of composition, and degradation mechanisms. Predictive tools should encompass all materials (metals, polymers, reinforced composites, filled polymers, advanced ceramics) to enable greater selection of new materials. They should permit forward and backwards modeling (be able to start with a material, see how can it be used, versus starting with an environment and predicting the best material).   A key element will be to integrate fitness-for-service with probability of detection and failure. New models should be able to design solutions for problems and could be used for condition assessment. Development of this capability will enable alloys by design and properties selection, and permit materials performance to be better incorporated in the design phase.

Technical Challenges

- Incomplete collection of thermodynamic and kinetic data for alloys and corrosives
- Insufficient process environmental data to predict alloy performance and/or degradation rates
- Lack of cost-effective technologies for on-line non-destructive evaluation
- Lack of standard polymer compounds
- Lack of standard format for data methods/content
- Lack of empirical data to build predictive models for many material/environment

Key R&D Elements

- Fundamental chemistry and thermodynamic models
- Fundamental models for corrosion behavior of alloys
- Fundamental understanding of polymer properties/interactions
- Fundamental understanding of coking, corrosion, stress cracking
- Expanded utility of existing alloy corrosion models (additional materials, localized corrosion)
- New non-destructive evaluation methods
- First principles modeling of degradation (e.g., high temperatures, liquid, permeation in polymers)
- Fast, high-precision measurement of property changes in non-metals exposed to corrosive environments
- Models for alloys–by-design that enable alloy development through prediction of mechanical and physical properties
- Measure and predict the rates of defect propagation
- Better fitness-for-service evaluation tools; better ways to identify and evaluate impacts of defects, stress
- Validation studies and a demonstration project

Partnership Roles and Responsibilities

Industry - Validation of models, guidance for R&D

Government - Funds pre-competitive R&D (e.g., DOE, DoD)

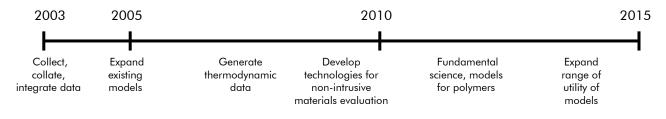**National Labs** - State-of-the-art resources, fundamental R&D

Universities – fundamental R&D, models

RISK

LOW   HIGH

Technical Risk

Model development is long term

Commercial Risk

Cost and demonstration will be a factor

BENEFITS

LOW   HIGH

Energy (mid-high)

Environment

Yield

Safety, Competitiveness, Flexibility, Reliability

Research Pathway

In the near-term, existing models will be expanded to increase capabilities and identify gaps. Collection, collation, and integration of a variety of materials and environmental performance data will be a key element. Generation of data and fundamental R&D will proceed in parallel with development of new measurement and monitoring technologies. The goal is to have reliable predictive capabilities that are commercially available and routinely used within 15 years. Government funding could reduce the risk of investment and accelerate R&D.

2003	2005		2010		2015
Collect, collate, integrate data	Expand existing models	Generate thermodynamic data	Develop technologies for non-intrusive materials evaluation	Fundamental science, models for polymers	Expand range of utility of models

Delivery of Materials Engineering Information

The grand challenge is to create a centralized information system containing comprehensive, standardized, refereed data and tools. This system would provide links to and be compatible with external tools and models. Ideally, it would be a "smart" database incorporating various layers and interpretation of data. The system will incorporate a search engine for materials data, and provide advice for materials selection as well as data mining. Information from "Masters" would be captured in the system, along with the capability to lead users to an expert if necessary.

Technical Challenges

- Poor quality data (e.g., obsolete, proprietary, non-reviewed (peer), inconsistent, incomplete)
- Loss of technical "Masters" with no replacement system
- Continuous changes in information technology
- Variance in company and industry needs
- Language and cultural diversity (global/local variations in data

Key R&D Elements

- International literature search to identify available data bases and define complete state-of-the-art
- Collect and collate data
- Effective system structure
- Use modern computer technology to cover/evaluate/link data in different disciplines
- Definition of customer needs up-front
- Methodical schematic of the system process using decision trees
- Initially populating the system with available high-value data (capture the low-hanging fruit)
- Materials engineers provide advice and input on interpretation of data
- Guidelines/rules for acceptable data
- Simple platforms to integrate data

Partnership Roles and Responsibilities

Industry – Provides data, design criteria, in-kind cost sharing. Includes IT companies, basic industries, equipment manufacturers.
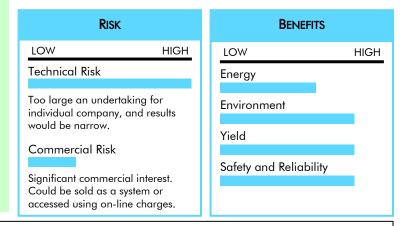
Government - Funds pre-competitive R&D (e.g., DOE, DOC, DoD). System could reside at DOC/NIST.

National Labs – Collect/collate data, assist with software/hardware development, screening/testing data.

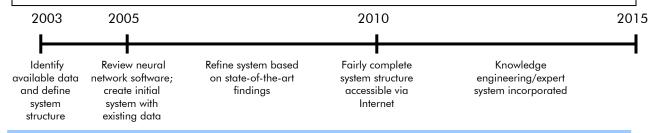**Universities** – Characterization of materials properties, provide advice.

RISK

LOW   HIGH

Technical Risk

Too large an undertaking for individual company, and results would be narrow.

Commercial Risk

Significant commercial interest. Could be sold as a system or accessed using on-line charges.

BENEFITS

LOW   HIGH

Energy

Environment

Yield

Safety and Reliability

Research Pathway

Initial efforts would identify what data and information systems are already available, and then define the structure of the proposed system. The objective is to have a well-defined materials engineering system structure in place by 2010. Knowledge engineering and interpretive capability would be incorporated by 2013. Smart system capabilities will develop as outlined in Chapter 3. Data will be added to the system on a continuous basis as new materials are developed and additional data becomes available.   Having the system reside at one of the national labs or DOC/NIST would be a huge advantage from an accessibility standpoint.

2003	2005		2010	2015
Identify available data and define system structure	Review neural network software; create initial system with existing data	Refine system based on state-of-the-art findings	Fairly complete system structure accessible via Internet	Knowledge engineering/expert system incorporated

Appendix

Technology Roadmap Participants

Jim Alexander, DuPont Dow Elastomers
John Aller, Capstone Engineering
Peter Angelini, Oak Ridge National Laboratory
Charlie Arnold, Dow Chemical
Sean Barnes, DuPont
Edward Blessman, Trent Tube
John Bringas, Casti Publishing
Juan Bustillos, Dow Chemical
Ed Clayton, Procter & Gamble (retired)
Gary Coates, Nickel Development Institute
Terry Cowley, DuPont
Bill Cox, Corrosion Management, Ltd.
Tom Crump, Consultant
Brian Fitzgerald, ExxonMobil Chemical Company
Emory Ford, Materials Technology Institute
Joseph Gates, An-Cor
Steve Grise, DuPont
Rolf Hansen, Norsk Hydro
Eric Harding, ExxonMobil Chemical Company
John Harnly, ExxonMobil Chemical Company
Dick Jones, Chemstress Consultant Company
Jeff Jones, ExxonMobil Chemical Company
Jim Kelly, Rolled Alloys
Pradip Khaladkar, DuPont
Gene Liening, Dow Chemical
Jim Macki, Materials Technology Institute
Bert Moniz, DuPont
Ed Naylor, Akzo Nobel
Joe Payer, Case Western Reserve University
Michael Renner, Bayer
Tony Richardson, Consultant (retired from ICI)
Melissie Rumizen, Buckman Laboratories
Sandy Sharp, MeadWestvaco
Mike Soboroff, U.S. Department of Energy
Charles Sorrell, U.S. Department of Energy
Steve Weiner, Pacific Northwest National Laboratory
Gary Whittaker, Eastman Chemical
Kelly Wyrough, Roben Manufacturing